

# FRACTIONAL COMBINATORIAL TREATMENT DESIGN

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# FRACTIONAL COMBINATORIAL TREATMENT DESIGN

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## ABSTRACT

Some theoretical and constructional results for the undeveloped subject of obtaining fractions from a complete combinatorial to estimate various mixing effects are presented. The complete set of  $m$  items taken  $n$  at a time is denoted as the combinatorial  $N = m!/n!(m - n)!$ . The desired fractional combinatorial should be minimal as well as optimal in order to have efficient fractions. Minimal fractional combinatorials are obtained for estimating general mixing ability, general plus bi-specific mixing abilities, and general plus bi-specific plus tri-specific mixing abilities. Some optimality results are presented.

Key words and phrases: diallel crossing, top-crossing, top-mixing,  $k$ -specific mixing ability, response model, minimal treatment design,  $t$ -designs, balanced incomplete block design, Latin square, Youden design

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## 1. INTRODUCTION

The set of all possible combinations of  $m$  items taken  $n$  at a time, i. e.,  $m!/n!(m - n)!$ , is denoted as a *combinatorial*. Any subset of a combinatorial is called a *fractional combinatorial*. Each combination of  $n$  items is known as a mixture of  $n$  items. Responses may or not be available for each item in a mixture. A variety of treatment effects are present in a mixture (See Federer, 1993, 1999, 2000). A *general mixing ability* (GMA) effect is an effect attributable to an item because it is in a mixture and is independent of which mixture it appears in. A GMA effect is different from the item effect appearing as a single (sole) item. The GMA effect plus the item effect as a sole entity is designated as an *item effect*. A *bi-specific mixing ability* (BSMA) effect is a two-item interaction effect for each pair of items. When individual responses are available, it is possible to obtain the contribution of each item to the interaction. This is in contrast to the usual factorial interaction situation. A *tri-specific mixing ability* (TSMA) effect is a three-item interaction effect and is available for all possible triplets of items. Again, if individual responses are available for each item in a mixture of three or more items, it is possible to estimate the contribution of each item to the interaction. A *quat-specific mixing ability* (QSMA) effect is a four-item interaction effect and is available for each quartet of the  $m$  items. A *k-specific mixing ability effect* is a  $k$ -item interaction effect.

Hall (1975) and Federer and Raghavarao (1987) presented minimal designs for  $n = k$  for estimating item effects and specific mixing ability effects up to KSMA effects. The treatment design is all possible combinations of  $m$  items taken  $k$  at a time. In many situations,  $k$  will be less than  $n$  and a fraction of the combinatorial will be desired. For example, an investigator may wish to use mixtures of size  $n = 4$  but is interested in item and BSMA effects, believing that TSMA and QSMA effects are negligible or non-existent. The question arises as to the minimal fraction of the combinatorial that can be used to obtain item and BSMA effects. It would be desirable to have the fraction optimal as well.

This paper deals with the construction of minimal treatment design (MTD) for various values of  $n$  for estimating GMA effects, for estimating GMA and BSMA effects, and for estimating item GMA, BSMA effects, and TSMA effects. If sole or single item treatments are not included, then only the item means (overall mean plus sole effect plus GMA) are estimable. Some results on optimal designs are presented also. Section 2 of the paper considers MTDs when individual item responses are available for each item in a mixture. Section 3 deals with MTDs for the case when only a mixture total response is available, the individual item responses are unobtainable. In this case an individual item's contribution to an interaction is not estimable. The BSMA interaction here is akin to specific combining ability interaction in diallel crossing experiments in genetic breeding studies.

## 2. INDIVIDUAL ITEM RESPONSES AVAILABLE

### 2.1. MTDs For Item Means and GMA Effects

A linear response may be of the form for sole item and the  $h$ th item in a mixture:

$$Y_{sg} = \mu_{sh} + \epsilon_{sgh} = \mu + \tau_h + \epsilon_{sgh} \quad \text{for the sole item} \quad (2.1.1)$$

$$Y_{mgh} = (\mu_{mh} + \epsilon_{mgh} = \mu + \tau_h + \delta_h + \epsilon_{mgh}) / n \quad \text{for the } h\text{th item in a mixture} \quad (2.1.2)$$

where  $\mu$  is a general mean effect,  $\tau_h$  is an effect of the  $h$ th item as a sole item,  $\delta_h$  is the GMA effect for the  $h$ th item,  $\mu_{xh}$  is the  $h$ th item mean for  $x = s$  or  $m$ , and  $\epsilon_{xgh}$  is a random error effect distributed with mean zero and common variance  $\sigma^2$ . The arithmetic mean for item  $h$  in a mixture minus its mean as a sole entity is an estimate of the  $h$ th item GMA effect, i. e.,  $\delta_h$ . The factor  $1/n$  is used to put the effects in (2.1.1) and (2.1.2) on the same basis as for a sole item. This assumes that an item is  $1/n$ th of the mixture. If the item in the mixture is the same as the sole item, then the factor  $1/n$  would be omitted (See Federer, 1993, 1999).

The addition of  $m$  sole items to the treatment design is necessary if GMA effects are desired. These may be omitted if only item means are desired. The rest of the paper is cast in terms of obtaining item means rather than GMA effects. The  $m$  sole items merely need to be added to the treatment design in order to estimate GMA effects also. The following theorem states how to form MTDs for estimating item means. Let  $v$  be the number of mixtures.

*Theorem 2.1.1.* MTDs for estimating item means may be constructed as follows:

- (i). The minimum number of mixtures is  $v = 1$  and is formed by taking one mixture of all  $m$  items.
- (ii).  $v = m/n$  to the next largest integer mixtures of sizes  $n = 2, 3, \dots, m$  may be formed by grouping items and duplicating some items if necessary.
- (iii). For  $m$  odd an incomplete block design arrangement of the  $m$  items in blocks of two may be formed from two rows of a cyclic Latin square to form  $v = m$  mixtures.
- (iv). A top-mixing design for  $v = m$  mixtures of each of the  $m$  items mixed with a standard item.

A response for each of the  $m$  items is sufficient to allow estimation of the item means. All of the above methods of construction supply at least one response for each of the  $m$  items. As an example of (ii), let  $m = 5$  and  $n = 2$ . Then the  $v = 3$  mixtures are (1, 2), (3, 4), and (5, 1). Incomplete blocks of size 2 for

an odd number of treatments allow estimation of the  $m$  item means from the mixture (block) totals. If  $m$  is even, the resulting circulant design matrix does not have an inverse. In top-crossing genetic experiments, each of  $m$  cultivars is crossed with a standard cultivar and the cross (mixture) is called a top-cross. Federer (2000) denotes this set-up for items as a top-mixing design and the mixture as a top-mix. Such a design is also part of a supplemented block design.

## 2.2. MTDs for Item Means and BSMA Effects

If item effects and BSMA effects are present, then response model equations for items  $h$ ,  $i$ , and  $j$  in the mixture  $hij$  may be (Federer, 1993, 1999):

$$Y_{gh(i,j)} = [\mu_{h(i,j)} + \varepsilon_{gh(i,j)} = \mu + \tau_h + \delta_h + 2(\gamma_{h(i)} + \gamma_{h(j)}) + \varepsilon_{gh(i,j)}] / (n=3) \quad (2.2.1)$$

$$Y_{gi(h,j)} = [\mu_{i(h,j)} + \varepsilon_{gi(h,j)} = \mu + \tau_i + \delta_i + 2(\gamma_{i(h)} + \gamma_{i(j)}) + \varepsilon_{gi(h,j)}] / 3 \quad (2.2.2)$$

$$Y_{gj(h,i)} = [\mu_{j(h,i)} + \varepsilon_{gj(h,i)} = \mu + \tau_j + \delta_j + 2(\gamma_{j(h)} + \gamma_{j(i)}) + \varepsilon_{gj(h,i)}] / 3 \quad (2.2.3)$$

where  $\gamma_{h(i)}$  is the BSMA effect for item  $h$  in the presence of item  $i$ ,  $h, i, j = 1, 2, \dots, m$ ,  $h \neq i \neq j$  and the remaining symbols are as defined above. The factor  $2/3$  is used to place the BSMA on the same basis as for a mixture of size  $n = 2$ . In order to obtain estimates of item means and BSMA effects, it is sufficient that the MTD contain  $m(m-1)$  responses and that the  $m(m-1)$  means  $y_{h(i,.)}$  be estimable. Then the item  $h$  mean is  $\bar{y}_{h(.,.)}$  and a BSMA effect for item  $h$  in the presence of item  $i$  is the difference of the two means,  $y_{h(i,.)} - y_{h(.,.)}$ .

MTDs may be constructed as follows:

*Theorem 2.2.1.* The minimum number of mixtures  $v = m(m-1)/n$  is obtained by using  $n = m-1$  and the MTD is formed by taking any  $m-1$  rows of an  $m$  by  $m$  Latin square and using the items in the columns as the  $v = m$  mixtures. This design is also optimal as the remaining items in a mixture for any item  $h$  form a BIBD for  $m-1$  items in  $m-1$  incomplete blocks of size  $m-2$ .

It is thought that the following theorem is true:

*Theorem 2.2.2.* If  $n > 3$ , if a BIBD for  $m$  treatments in  $v$  distinct incomplete blocks of size  $n$  for  $\lambda = n-1$  exists, if an incomplete block design for the remaining  $m-1$  treatments for each treatment exists, and if  $m > 4$ , then a MTD for item means and BSMA effects may be constructed using this BIBD.

## 2.3. MTDs For Item Means, BSMA Effects and TSMA Effects.

A response model equation for the  $h$ th item in the mixture  $hijk$  may be written as

$$Y_{gh(i,j,k)} = [\mu_{h(i,j,k)} + \varepsilon_{gh(i,j,k)} = \mu + \tau_h + \delta_h + 2(\gamma_{h(i)} + \gamma_{h(j)} + \gamma_{h(k)}) + 3(\pi_{h(i,j)} + \pi_{h(i,k)} + \pi_{h(j,k)} + \varepsilon_{gh(i,j,k)})] / n=4 \quad (2.3.1)$$

where  $\pi_{h(i,j)}$  is the contribution of item  $h$  to the three factor interaction of items  $h, i$ , and  $j$ . This is denoted as a TSMA effect for item  $h$  in the presence

of items  $i$  and  $j$ . The other symbols have been defined previously. The number of responses required to estimate the item means, the BSMA effects and the TSMA effects is  $m(m-1)(m-2)/2$ . The minimum number of mixtures of size  $n$  required is  $v = m(m-1)(m-2)/2n$ . An example of an MTD for  $m = 6$  and  $n = 4$  is given in Appendix 2.3. This design is also optimal as  $v = m! / n! (m-n)!$  and a BIBD of the remaining treatments in the mixture results for each pair of items. The following procedures may be used to construct MTDs. The problem is to estimate the  $(m-2) \mu_{h(i,j,.)}$  means for each pair  $ij$ , and from these, estimates of the BSMA  $= \gamma_{h(i)} = \mu_{h(i,.,.)} - \mu_{h(.,.,.)}$  and TSMA  $= \pi_{h(i,j)} = \mu_{h(i,j,.)} - [\mu_{h(i,.,.)}]$  effects are obtained. This requires that  $\mu_{h(i,j,.)}$  is estimable for each of the possible pairs  $ij$ .

One method of constructing MTDs is illustrated in the following example for  $m = 8$ ,  $n = 4$ , and  $v = 42$ . Starting with a cyclic  $8 \times 8$  Latin square, select the first four rows to obtain the eight mixtures 1 to 8. Then select rows 1, 2, 5, and 6 of the Latin square to obtain mixtures 9 to 16. Select rows 1, 2, 7, and 8 of the Latin square to form mixtures 17 to 24. Use rows 1, 4, 5, and 7 to obtain mixtures 25 to 32. Rows 1, 3, 4, and 6 are used to obtain mixtures 33 to 40. Note that this selection of quartets of rows results in distinct mixtures of four items. To form mixtures 41 and 42, use the mixtures 1, 3, 5, 7 and 2, 4, 6, 8. The resulting 42 distinct mixtures are:

```

1 2 3 4 5 6 7 8  1 2 3 4 5 6 7 8  1 2 3 4 5 6 7 8  1 2 3 4 5 6 7 8  1 2 3 4 5 6 7 8  1 2
2 3 4 5 6 7 8 1  2 3 4 5 6 7 8 1  2 3 4 5 6 7 8 1  4 5 6 7 8 1 2 3  3 4 5 6 7 8 1 2  3 4
3 4 5 6 7 8 1 2  3 4 5 6 7 8 1 2  5 6 7 8 1 2 3 4  5 6 7 8 1 2 3 4  4 5 6 7 8 1 2 3  5 6
4 5 6 7 8 1 2 3  5 6 7 8 1 2 3 4  7 8 1 2 3 4 5 6  7 8 1 2 3 4 5 6  6 7 8 1 2 3 4 5  7 8

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Although this 42 / 70 fractional combinatorial plan is a MTD, it is not optimal as the design matrix  $X$  for any pair  $hi$  has between 7 and 11 associated responses instead of nine for every pair. It is possible to construct a BIBD for this example. The software package GENDEX is one such package for constructing incomplete block designs. These may be constructed using the BIB or the CIB module in the package. A particular BIBD generated from the BIB module is (Note that each run produces a different plan and that repeated blocks may occur.):

```

1 1 1 1 1 1 1 1  1 1 1 1 1 1 1 1  1 1 1 1 1 2 2 2  2 2 2 2 2 2 2 2  2 3 3 3 3 3 3 4  4 4
2 2 2 2 2 2 2 2  2 3 3 3 3 3 3 4  4 4 5 5 5 3 3 3  3 3 3 4 4 4 5 5  5 4 4 4 5 6 6 5  6 6
3 3 3 4 4 4 6 6  6 4 4 4 5 5 7 5  5 5 6 6 7 4 4 4  5 5 5 5 6 7 6 7  7 5 5 6 6 7 7 6  7 7
6 8 8 5 7 8 7 7  8 6 7 8 6 7 8 6  7 8 7 8 8 5 6 7  6 7 8 6 8 8 7 8  8 7 8 7 8 8 8 8  8 8

```

Note that blocks (mixtures) (1,2,3,8), (1,2,6,7), (2,5,7,8), (3,6,7,8), and (4,6,7,8) are repeated blocks. For this plan, not all  $\mu_{h(i,j,.)}$  are estimable, e.g., the pairs 68 and 78 have an  $X'X$  which has rank 5 instead of the required 6.

A plan generated by the CIB module has 42 distinct blocks and is:

```

1 1 1 1 1 1 1 1  1 1 1 1 1 1 1 1  1 1 1 1 1 2 2 2  2 2 2 2 2 2 2 2  2 3 3 3 3 3 3 4  4 5
2 2 2 2 2 2 2 2  2 3 3 3 3 3 3 4  4 4 4 5 6 3 3 3  3 3 3 4 4 4 4 5  5 4 4 4 4 5 5 5  5 6
3 3 3 4 4 5 5 6  7 4 4 5 5 5 6 5  5 6 7 6 7 4 4 5  5 6 7 5 6 6 7 6  6 5 5 6 6 6 7 6  7 7
4 6 8 5 6 7 8 7  8 7 8 6 7 8 7 6  7 8 8 8 8 5 7 6  7 8 8 8 7 8 8 7  8 6 8 7 8 8 8 7  8 8

```

BIBD plans exist for  $m$  items in mixtures of size  $n$  when  $m(m-1)(m-2)/2 = nv$ , or when  $v = m(m-1)(m-2)/2n$ . Thus,  $m$  is required to be even when  $n = 4$ . The number of times each pair of items occurs in a mixture is  $\lambda = (n-1)(m-2)/2$ .

*Theorem 2.3.1.* An MTD for  $m$  items in mixtures of size  $n$  for estimating item means, BSMA effects, and TSMA effects may be obtained from a incomplete block

design for  $m$  items in mixtures of size  $n$  with  $r = (m - 1)(m - 2) / 2$  replicates in  $v = m(m - 1)(m - 2) / 2n$  distinct mixtures (blocks) if for each pair of items the incomplete block design for the remaining items is connected. If this incomplete block design is also a BIBD, the MTD is also optimal.

We need  $m(m - 1)(m - 2)/2 = vn$  as well as pairwise balance of  $\lambda = (m - 2)(n - 1) / 2$ . This limits values of  $m$ . The following "theorem" may not be true as stated but one should be able to construct a MTD with minimum  $v$  by this method. Perhaps in forming the cube the sides must be orthogonal also.

*Theorem 2.3.2.* An MTD with the minimum number of mixtures  $v$  may be obtained starting with a Latin cube of order  $m$  and using deletions by first cutting the cube in half diagonally, using the items below (or above) the cut, deleting two layers, and using items in the columns of the remaining  $m - 2$  layers to form  $m(m - 1) / 2$  mixtures of size  $m - 2$ . The number of items  $m > 7$ .

To illustrate consider the following Latin cube of order six (the procedure works for any  $m$ ):

1 2 3 4 5 6	2 3 4 5 6 1	3 4 5 6 1 2	4 5 6 1 2 3	5 6 1 2 3 4	6 1 2 3 4 5
2 3 4 5 6 1	3 4 5 6 1 2	4 5 6 1 2 3	5 6 1 2 3 4	6 1 2 3 4 5	1 2 3 4 5 6
3 4 5 6 1 2	4 5 6 1 2 3	5 6 1 2 3 4	6 1 2 3 4 5	1 2 3 4 5 6	2 3 4 5 6 1
4 5 6 1 2 3	5 6 1 2 3 4	6 1 2 3 4 5	1 2 3 4 5 6	2 3 4 5 6 1	3 4 5 6 1 2
5 6 1 2 3 4	6 1 2 3 4 5	1 2 3 4 5 6	2 3 4 5 6 1	3 4 5 6 1 2	4 5 6 1 2 3
6 1 2 3 4 5	1 2 3 4 5 6	2 3 4 5 6 1	3 4 5 6 1 2	4 5 6 1 2 3	5 6 1 2 3 4

The cube is cut diagonally and the parts below the cut are retained as follows:

2	3	4	5	6	1
3 4	4 5	5 6	6 1	1 2	2 3
4 5 6	5 6 1	6 1 2	1 2 3	2 3 4	4 5 6
5 6 1 2	6 1 2 3	1 2 3 4	2 3 4 5	3 4 5 6	4 5 6 1
6 1 2 3 4	1 2 3 4 5	2 3 4 5 6	3 4 5 6 1	4 5 6 1 2	5 6 1 2 3

Delete two layers, say the last two. Then, stack the layers  $m - 2$  deep and the items in a column form the  $m(m - 1) / 2$  mixtures of size  $4 = m - 2$ . The resulting MTD has the minimum number of mixtures  $v$  to estimate the item means, the BSMA effects, and the TSMA effects and is:

2	3 4	4 5 6	5 6 1 2	6 1 2 3 4
3	4 5	5 6 1	6 1 2 3	1 2 3 4 5
4	5 6	6 1 2	1 2 3 4	2 3 4 5 6
5	6 1	1 2 3	2 3 4 5	3 4 5 6 1

(This is not an MTD allowing estimation of the desired effects but I think using  $m = 7$  and having the Latin squares on the sides of the cube orthogonal would work.)

### 3. ONLY MIXTURE TOTALS AVAILABLE

#### 3.1 MTDS For Item Means

When responses for individual items in a mixtures are not available, i.e., only mixture totals are obtainable, a response model equation for a mixture is given below. To estimate the item means,  $m$  distinct mixtures are required. These may be obtained as top-mixes or by using an incomplete block design for  $m$  mixtures of size  $n$ . For  $n = 2$  and  $m$  even, items cannot be estimated as a

circulant design matrix results. The response model equations for item means for  $n = 2, 3$ , and  $4$  as considered by Federer (1999) are (blocking effect parameter omitted and  $\beta_h$  is an item or cultivar effect):

$$Y_{ghi} = \mu_{hi} + \epsilon_{ghi} = \mu + (\beta_h + \beta_i)/2 + \epsilon_{ghi} \quad (3.1.1)$$

$$Y_{ghij} = \mu_{hij} + \epsilon_{ghij} = \mu + (\beta_h + \beta_i + \beta_j)/3 + \epsilon_{ghij} \quad (3.1.2)$$

$$Y_{ghijk} = \mu_{hijk} + \epsilon_{ghijk} = \mu + (\beta_h + \beta_i + \beta_j + \beta_k)/4 + \epsilon_{ghijk} \quad (3.1.3)$$

Solutions for item means equal to  $\mu_{h...} = \mu + \beta_h/n$  are needed. The factor  $1/n$  is used to put the item effects,  $\beta_h$ , on the same basis as a sole mixture.

### 3.2. MTDs For Item Means and BSMA Effects

Response model equations for item effects and BSMA effects in mixtures of sizes  $n = 2, 3$ , and  $4$  as given by Federer (1999) are:

$$Y_{ghi} = \mu_{hi} + \epsilon_{ghi} = \mu + (\beta_h + \beta_i)/2 + \gamma_{hi} + \epsilon_{ghi} \quad (3.2.1)$$

$$Y_{ghij} = \mu_{hij} + \epsilon_{ghij} = \mu + (\beta_h + \beta_i + \beta_j)/3 + 2(\gamma_{hi} + \gamma_{hj} + \gamma_{ij})/3 + \epsilon_{ghij} \quad (3.2.2)$$

$$Y_{ghijk} = \mu_{hijk} + \epsilon_{ghijk} = \mu + (\beta_h + \beta_i + \beta_j + \beta_k)/4 + 2(\gamma_{hi} + \gamma_{hj} + \gamma_{hk} + \gamma_{ij} + \gamma_{ik} + \gamma_{jk})/4 + \epsilon_{ghijk} \quad (3.2.3)$$

where  $\gamma_{hi}$  is the interaction or BSMA effect for the pair  $hi$  and the remaining symbols are as defined above. There are  $m(m-1)/2$  means  $\mu_{hi...}$  to be estimated. For each  $h$ , the  $m-1$   $\mu_{hi}$  must be estimable. An estimate of  $\mu_{hi...}$  is the estimated item mean, and an estimate of  $\gamma_{hi} = \mu_{hi...} - \mu_{h...}$  is the estimated BSMA effect. The number of independent responses and the number of mixtures required is  $v = m(m-1)/2$ . Thus a fraction of at least  $n!(m-n)!/2(m-2)!$  of the total number of mixtures  $N = m!/n!(m-n)!$  is required. Federer (1999) gives a numerical example of a  $6/8$  fraction of  $6!/3!(6-3)! = 20$  mixtures to estimate item means and BSMA effects for  $m = 6$ .

Consider the following plan for  $m = 9$  items, mixtures of size  $n = 3$ , and  $v = 36$  mixtures which is equal to  $9(8)/2$ , the number of responses required. The plan is a BIBD for  $m = 9$ ,  $n = 3$ ,  $r = 12$ , and  $\lambda = 3$ .

1 1 1 1 1 1	1 1 1 1 1 1	2 2 2 2 2 2	2 2 2 3 3 3	3 3 3 4 4 4	4 4 5 5 6 6
2 2 2 3 3 3	4 5 5 5 7 7	3 3 3 4 4 5	6 6 8 4 4 5	5 6 7 5 5 6	7 8 6 7 7 8
4 6 8 4 7 9	6 6 8 9 8 9	5 7 9 5 8 7	7 9 9 6 8 6	9 8 8 7 9 7	9 9 8 8 9 9

For each  $h$ , it is possible to obtain solutions for  $\mu_{hi..}$  for  $h \neq i = 1, \dots, 9$ . Plans for  $m = 9$  and  $n = 4, 5$ , and  $6$  are given in Appendix C.

**Theorem 3.2.1.** A BIBD for  $m$  items in  $v$  distinct mixtures of size  $n$  with  $r = n(m-1)/2$  replicates, and  $\lambda = n(n-1)/2$  is sufficient to construct the  $v = m(m-1)/2$  mixtures for estimating item means and BSMA effects.

**Corollary 3.2.1.** A necessary condition is that  $r$  minus the number of times blocks are repeated,  $rb$ , for each  $h$  must be greater than or equal to  $m-1$  in order to estimate the  $\mu_{hi...}$ .

If  $r - r_b < m - 1$ , the rank of the design matrix will be less than the required  $m - 1$ .

### 3.3. MTDs For Item Means, BSMA Effects, and TSMA Effects

Response model equations for mixtures of  $n = 3$  and  $4$  when item, BSMA, and TSMA effects are present as presented by Federer (1999) are:

$$Y_{ghij} = \mu_{hij} + \varepsilon_{ghij} = \mu + (\beta_h + \beta_i + \beta_j)/3 + 2(\gamma_{hi} + \gamma_{hj} + \gamma_{ij})/3 + \pi_{hij} + \varepsilon_{ghij} \quad (3.3.1)$$

$$Y_{ghijk} = \mu_{hijk} + \varepsilon_{ghijk} = \mu + (\beta_h + \beta_i + \beta_j + \beta_k)/4 + 2(\gamma_{hi} + \gamma_{hj} + \gamma_{hk} + \gamma_{ij} + \gamma_{ik} + \gamma_{jk})/4 + 3(\pi_{hij} + \pi_{hik} + \pi_{hjk} + \pi_{ijk})/4 + \varepsilon_{ghijk} \quad (3.3.2)$$

where the  $\pi_{hij}$  is the three factor  $hij$  interaction effect and the other symbols are as defined previously. The factors  $2/3$  and  $2/4$  represent the proportion of the mixture devoted to a BSMA effect. The factor  $3/4$  represents the proportion of the mixture available for a TSMA effect. The number of means  $\mu_{hij\dots}$  to be estimated is  $m! / 3! (m - 3)! = m(m - 1)(m - 2) / 6$ , and this is the number of responses as well as the number of mixtures  $v$  that are required. If  $N = m! / n!(m - n)!$ ,  $n > 3$ , a saturated fractional combinatorial for the above response models is a  $v / N$  fraction of  $N$ .

*Theorem 3.3.1.* A MTD for estimating item means, BSMA effects, and TSMA effects may be obtained from a BIBD for  $m$  items in distinct mixtures (blocks) of size  $n$  with  $n(m - 1)(m - 2) / 6$  replicates and  $\lambda$  (an integer)  $= n(m - 2)(n - 1) / 6$ .

## 4. DISCUSSION AND SOME UNSOLVED PROBLEMS

As indicated above, there are many fractions for which BIBDs do not exist. Also to have saturated fractions, unequal replication of items may be required for some  $m$  and  $n$ . If QSMA effects are also desired, how does one construct such a fraction? Are there procedures for constructing minimal and optimal treatment designs? What are they?

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APPENDIX 2.2 - MTD plans for Section 2.2; item means and BSMA effects from BIBDs for  $m$  items in  $v$  incomplete blocks of size  $n$  with  $m - 1$  replicates.

$m = 5, n = 2, v = 10$	0 0 0 0 1 1 1 2 2 3 (m = 5)! / 2!(5 - 2)!)
	1 2 3 4 2 3 4 3 4 4
$m = 5, n = 4, v = 5$	0 1 2 3 4 (4 rows of a 5x5 Latin square, v minimal)
	1 2 3 4 0
	2 3 4 0 1
	3 4 0 1 2
$m = 8, n = 4, v = 14$	0 0 0 0 0 0 0 1 1 1 1 2 2 4
	1 1 1 2 2 3 4 2 2 3 3 3 3 5
	2 3 4 6 3 5 5 4 5 6 4 4 5 6
	5 7 6 7 4 6 7 7 6 7 5 6 7 7
$m = 9, n = 4, v = 18$	0 0 0 0 0 0 0 0 1 1 1 1 1 2 2 2 3 4
	1 1 1 2 2 3 4 5 2 2 3 3 4 3 3 5 5 5
	2 3 4 3 7 4 6 6 4 5 6 7 6 4 4 6 6 7
	7 5 5 6 8 8 8 7 6 8 8 8 7 5 7 8 7 8
$m = 9, n = 6, v = 12$	0 0 0 0 0 0 0 0 1 1 1 2
	1 1 1 1 1 2 2 3 2 2 3 4
	2 2 2 3 5 3 3 4 3 3 4 5
	3 4 4 4 6 4 5 5 4 6 5 6
	5 5 6 6 7 7 6 6 5 7 7 7
	8 7 8 7 8 8 7 8 6 8 8 8
$m = 10, n = 6, v = 15$	0 0 0 0 0 0 0 0 0 1 1 1 1 2 3
	1 1 1 1 1 2 2 2 3 2 2 2 3 4 4
	2 2 3 4 5 3 3 4 4 3 3 4 5 5 6
	3 6 4 6 7 6 5 5 5 4 5 5 6 6 7
	4 7 5 7 8 8 7 6 7 7 6 8 8 7 8
	9 9 6 8 9 9 8 8 9 8 7 9 9 9 9
$m = 11, n = 5, v = 22$ (x = 11)	0 0 0 0 0 0 0 0 0 1 1 1 1 1 2 2 2 2 3 3
	1 1 1 1 2 2 3 3 4 6 2 2 3 4 5 5 3 3 4 4
	2 2 3 4 4 7 5 6 5 8 3 4 5 7 6 6 4 6 5 6
	3 7 4 8 5 8 9 7 7 9 7 6 8 9 8 7 9 8 8 7
	5 8 6 9 6 x x 9 x x 9 x x x 9 x x x 9 9 8 8

APPENDIX 2.3 - MTDs for Section 2.3; item means, BSMA effects, and TSMA effects.

$m = 6, n = 4, v = 15$	1 1 1 1 1 1 1 1 1 2 2 2 2 3
	2 2 2 2 2 3 3 3 4 3 3 3 4 4
	3 3 3 4 4 5 4 4 5 5 4 4 5 5
	4 5 6 5 6 6 5 6 6 5 6 6 6 6

Some BIBDs that may be generated by GENDEX are given below. These may be used as MTDs for estimating item means, BSMA effects, and TSMA effects. (GENDEX gives BIBDs with repeated blocks many times. Sometimes a run will give distinct blocks which is preferred.)

Items =  $m$     Replicate     $v = m(m-1)$     Mixture

	number	$(m-2)/2$	size = n	$\lambda$
6	10	20	3	4
	10	15	4	6
7	15	35	3	5
	15	21	5	10
8	21	56	3	6
	21	42	4	9
	21	28	5	12
	21	24	6	15
9	28	84	3	7
	28	36	7	21
10	36	120	3	8
	36	90	4	12
	36	72	5	16
	36	60	6	20
	36	45	8	28
11	45	165	3	9
	45	99	5	18
	45	55	9	36
12	55	220	3	10
	55	165	4	15
	55	132	5	20
	55	66	10	45
13	66	286	3	11
	66	78	11	65
14	78	364	3	12
	78	273	4	18
	78	182	6	30
	78	91	12	72
15	91	455	3	13
	91	273	5	26
	91	195	7	39
	91	105	13	78

#### APPENDIX 3.2 - MTDs for Section 3.2; item means and BSMA effects

$m = 9, n = 4, v = 36$  (blocks distinct)

```

1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 2 2 2 2 2 2 2 2 2 2 2 3 3 3 3 3 3 4 4 4 5
2 2 2 2 2 2 3 3 3 3 4 4 4 5 5 6 3 3 3 3 4 4 4 4 5 6 4 5 5 5 6 7 5 6 6 7
3 3 5 5 6 7 4 4 4 5 6 7 8 6 7 8 4 4 6 7 5 5 5 6 7 7 5 6 6 7 8 8 6 7 8 8
6 8 8 9 8 9 5 7 8 6 7 9 9 7 9 9 7 9 9 9 6 8 9 7 8 8 8 7 8 9 9 9 9 8 9 9

```

$m = 9, n = 5, v = 36$  (blocks distinct)

```

1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 2 2 2 2 2 2 2 2 2 2 3 3 3 3 4 4
2 2 2 2 2 2 2 2 2 2 3 3 3 3 3 3 4 4 5 5 3 3 3 3 3 3 4 4 5 6 4 4 4 5 5 5

```

3 3 3 3 4 4 4 4 5 7 4 4 4 5 5 6 5 6 6 6 4 4 4 5 5 6 5 5 7 7 5 6 7 6 6 6  
 4 5 6 6 5 6 7 7 6 8 5 5 6 6 7 8 8 7 7 8 5 6 8 7 7 8 6 6 8 8 8 7 8 7 7 7  
 5 7 8 9 8 9 8 9 7 9 7 9 7 8 8 9 9 8 9 9 6 7 9 8 9 9 8 9 9 9 8 9 9 8 9

For  $m = 9$ ,  $n = 6$ ,  $v = 36$ , the designs obtained so far have repeated blocks and hence may not be MTDs.

### APPENDIX 3.3 - MTDs for Section 3.3; item means, BSMA effects, and TSMA effects.

BIBDs for  $v = m(m - 1)(m - 2) / 6$  mixtures of size  $n$  are listed below. These plans will need to have distinct blocks.

Items = m	Replicate Number	Number $v = n(m-1)(m-2)/6$	Mixture size = n	$\lambda$
6	10	20	3	4
7	15	35	3	5
	20	35	4	10
8	21	56	3	6
	28	56	4	12
	35	56	5	20
	42	56	6	30
9	28	84	3	7
10	36	120	3	8
	48	120	4	16
	72	120	6	40
	84	120	7	56
11	45	165	3	9
	75	165	5	18
12	55	220	3	10
	110	220	6	50
13	66	286	3	11
	88	286	4	22
	132	286	6	55
14	78	364	3	12
	104	364	4	24
	130	364	5	40
	156	364	6	60
	182	364	7	84
	208	364	8	112
	234	364	9	144
	260	364	10	180
	286	364	11	220
	312	364	12	264
15	91	455	3	13
	182	455	6	26
	273	455	9	39
	364	455	12	52